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# Analysis of PCA-based reconstruction method for fault diagnosis

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## Abstract

The reconstruction method, defined in the frame of principal component analysis, is a popular and representative method for fault diagnosis. It has been successfully applied in several industrial processes. Although the sufficient condition of the uniquely fault subspace identification has been provided in literature, it cannot be used in practice due to the true fault subspace and magnitude is unknown. Thus this condition cannot be used to confirm whether an identified subspace is the true fault subspace once there are more than one subspace determined as the possible candidates. This paper shows that the true fault subspace is hard to be identified **when a fault occurred and caused a significant change in the correlation of the variables while the**

**$T^2$  index is still in control.** Through the theoretical analysis and some illustrative examples, it is shown that the reconstruction method cannot always uniquely identify the true fault subspace in these cases. This indicates that care must be taken when using the reconstruction method. Some possible solutions are also provided in order to further improve the reconstruction method.

## Introduction

Statistical process monitoring applies multivariate statistical methods such as principal component analysis (PCA) to the fault diagnosis of industrial processes.<sup>1-3</sup> PCA divides the measurement space into the principle component subspace (PCS) and the residual subspace (RS).<sup>4</sup> For the detection of a new incoming sample, it is first projected onto the PCS and RS, respectively. Then, fault detection indices are calculated based on these projections. If one of the indices exceeds its control limit or threshold, the sample is considered as a faulty sample and the process may have an abnormal behavior. The widely used fault detection indices are the Hotelling's  $T^2$  statistic and the squared prediction error ( $SPE$ ) statistic.<sup>3</sup> Raich et al.<sup>5</sup> and Yue et al.<sup>6</sup> also developed the combined indices that incorporate the  $T^2$  and  $SPE$  statistics in order to facilitate the fault detection.

Once a fault is detected, it is desirable to diagnose the true faulty variables or subspace. An early and classical method for the identification of faulty variables is contribution plot<sup>7</sup> that associates each variable with a contribution quantity, which represents the amount of contributions of individual variables on the monitoring statistics. The one with the largest contribution is regarded as the faulty variable. Later, several contribution-based fault diagnosis methods, inspired by the idea of contribution plot, have been proposed.<sup>4,5,8,9</sup> These methods give different definitions for the variable contributions, and they were called contribution analysis methods (CAMs). These CAMs diagnose the faulty variables without using any historical fault data. Alcalá et al.<sup>4</sup> and Kerkhof et al.<sup>10</sup> presented comprehensive reviews of these methods.

A basic requirement for fault diagnosis is to avoid misdiagnosis as much as possible. However, the traditional contribution plot suffers from fault smearing effect,<sup>11</sup> which means the contribution quantity of non-faulty variables is liable to be enlarged by the faulty variables, thus can lead to misdiagnosis. This is because the linear transformation involved in the PCA model is inevitable in constructing of the variable contribution. Alcalá and Qin<sup>9</sup> indicated that these CAMs all suffer from the effect of fault smearing. However, Alcalá and Qin<sup>9</sup> proved that one of the CAMs, i.e., reconstruction-based contribution (RBC), can guarantee providing a correct result in the case of unidimensional fault with large magnitude though suffering from the fault smearing. This means the amount of RBC from the faulty variable may larger than that of other non-faulty variables. In order to improve the diagnosis accuracy, Xu et al.<sup>12</sup> proposed weighted RBC method that can reduce the effect of fault smearing. Liu et al.<sup>13,14</sup> proposed modified contribution plots based on missing data approach, which greatly reduces the smearing effect on non-fault variables. Alcalá and Qin<sup>15</sup> extended the RBC method with kernel PCA to diagnose nonlinear processes. Li et al.<sup>16</sup> also extended the RBC method to diagnose the output relevant faults based on the total projection to the latent structures (T-PLS) under the assumption that the fault directions is known. When multidimensional faults occur, Kerkhof et al.<sup>10</sup> have proved that the RBC method as well as the other CAMs cannot guarantee identifying the true faulty variables or subspace. Li et al.<sup>17</sup> proposed the multi-directional RBC method to diagnose the root-cause of the dynamic processes. Recently, in order to improve the ability of the RBC method in dealing with the more complex fault, Mnassri et al.<sup>18</sup> proposed a generalized RBC and RBC ratio to handle the more complex fault that occurs in multidimensional directions and remedy the defective of the RBC method.

Actually, the RBC method combines the idea of contribution plot with the reconstruction method<sup>17,19,20</sup> which is the core part of it. Fault diagnosis based on the reconstruction method was originally proposed by Dunia and Qin<sup>19,20</sup> using the *SPE* detection index. It is assumed that the faults affect a set of variables, i.e.,  $r(r < m)$ , and can be reconstructed

from the other  $m - r$  fault-free variables. The reconstruction method estimates the normal sample vector using the faulty or corrupted sample and the established PCA model, i.e., to reconstruct the normal operating conditions. Fault subspace identification is to find the true fault from a set of possible faults  $\mathcal{F}$ . It can be done by assuming each of the faults in  $\mathcal{F}$  in turn and performing the reconstruction.<sup>19</sup> If the true fault subspace is selected, the detection index of the reconstructed sample must be smaller than the control limit. If there is only one identified fault subspace, then the true fault is uniquely determined.<sup>6</sup> Otherwise, the true fault subspace cannot be uniquely identified.

Yue and Qin<sup>6</sup> extended the reconstruction method using the combined detection index and provided some theoretical results about its reconstructability and identifiability. Mnassri et al.<sup>21</sup> generalized the analysis to the more general quadratic index, thus the  $T^2$ ,  $SPE$ , or combined index can be seen as a special form of the general quadratic index. They also presented the sufficient conditions for the fault isolability based on the reconstruction method. The true fault subspace can be uniquely identified by the reconstruction method if the fault isolability condition is satisfied. However, the true fault subspace and magnitude is unknown in practice, so this condition cannot be used to confirm whether the identified fault subspace contradicts with the isolability condition or not.

In this paper, we briefly review the PCA based reconstruction method for fault diagnosis. We mainly analyzing the reconstruction method with a combined index proposed by Yue and Qin.<sup>6</sup> Because, on the one hand, the reconstruction method is a representative method and the core part of several PCA-based fault diagnosis methods. It can simultaneously realize the identification of faulty subspace and the estimation of fault magnitude. On the other hand, the reconstruction method using the combined index can identify some faults that uniquely using the  $SPE$  or  $T^2$  may not. The reconstruction methods have been applied to diagnose various industrial processes.<sup>17,22-24</sup> These achievements all show that the reconstruction-based fault diagnosis method is very powerful and effective. However, through the theoretical analysis and numerical simulations, we show that the reconstruction method

with a combined index cannot uniquely identify the fault subspace in some cases. **It is likely to occur when the fault affects one or several measured variables simultaneously causing significant changes in the variable correlation while the  $T^2$  index is still in control.** To reconstruct the normal sample and recover the variables correlation, it can be realized by modifying either these faulty variables or the other fault-free variables. In this case, the faulty sample vector can be brought back into the normal region using at least two subspaces, so it is hard to identify the true fault subspace. This reminds us to be careful when using the reconstruction method. Moreover, some possible solutions for this problem are also provided in order to further improve the reconstruction method.

## Statistical Process Monitoring

### Fault detection based on PCA

Consider a normal process historical data set consisting of  $n$  measurements with  $m$  variables and is arranged in a data matrix,  $\mathbf{X} \in \mathbb{R}^{n \times m}$ . Then,  $\mathbf{X}$  is scaled to zero-mean and unit variance for each variable, i.e. auto-scaled. For the remainder of this paper, the data are assumed to be auto-scaled. The PCA-based fault detection approaches require that the normal data  $\mathbf{X}$  should be rich in normal variations to be representative to the common-cause variability of the process.<sup>3</sup> PCA tries to find the directions called the principal components that have the maximum variability and can provide more parsimonious description of the covariance structure of  $\mathbf{X}$ .<sup>25</sup> The principal components can be obtained from eigen-decomposition of the covariance matrix,  $\mathbf{S}$ ,

$$\mathbf{S} = \frac{1}{n-1} \mathbf{X}^T \mathbf{X} = [\mathbf{P} \ \tilde{\mathbf{P}}] \begin{bmatrix} \mathbf{\Lambda} & \mathbf{0} \\ \mathbf{0} & \tilde{\mathbf{\Lambda}} \end{bmatrix} [\mathbf{P} \ \tilde{\mathbf{P}}]^T \quad (1)$$

where the columns of  $\mathbf{P} \in \mathbb{R}^{m \times l}$  are composed of the eigenvectors of  $\mathbf{S}$  associated with the first  $l$  largest eigenvalues contained in the diagonal matrix,  $\mathbf{\Lambda} \in \mathbb{R}^{l \times l}$ , in descending

order, while the remaining eigenvectors and eigenvalues contain in  $\tilde{\mathbf{P}} \in \Re^{m \times (m-l)}$  and the diagonal matrix  $\tilde{\mathbf{\Lambda}} \in \Re^{(m-l) \times (m-l)}$ , respectively. The columns of  $\mathbf{P}$  and  $\tilde{\mathbf{P}}$  span the principal component subspace (PCS) and the residual subspace (RS), respectively. The projection of a new incoming sample  $\mathbf{x}$  onto PCS and RS are

$$\begin{aligned}\hat{\mathbf{x}} &= \mathbf{P}\mathbf{P}^T\mathbf{x} = \mathbf{C}\mathbf{x} \\ \tilde{\mathbf{x}} &= \tilde{\mathbf{P}}\tilde{\mathbf{P}}^T\mathbf{x} = \tilde{\mathbf{C}}\mathbf{x}\end{aligned}\tag{2}$$

where  $\mathbf{C} = \mathbf{P}\mathbf{P}^T$  and  $\tilde{\mathbf{C}} = \tilde{\mathbf{P}}\tilde{\mathbf{P}}^T$  are symmetric and idempotent matrices.

When a fault occurs in a subspace  $\Xi_i$ , the resulted faulty sample can be represented as<sup>6</sup>

$$\mathbf{x} = \mathbf{x}^* + \Xi_i \mathbf{f}\tag{3}$$

where  $\mathbf{x}^*$  represents the part of fault-free measurement. The matrix  $\Xi_i \in \Re^{m \times l_i}$ , which is composed of any  $l_i$  ( $l_i < m$ ) columns of the  $m$ -dimensional identity matrix, represents the actual fault subspace. The vector  $\mathbf{f} \in \Re^{l_i}$  represents the fault magnitude.

Fault detection is achieved by comparing the statistical indices of a measurement  $\mathbf{x}$  with their control limits. The most commonly used indices are the squared prediction error, Hotelling's  $T^2$  and a combined index of them.<sup>26</sup>

The *SPE* index is defined as the squared  $l_2$  norm of the residual vector

$$SPE(\mathbf{x}) = \|\tilde{\mathbf{C}}\mathbf{x}\|^2 = \mathbf{x}^T \tilde{\mathbf{C}}\mathbf{x}\tag{4}$$

The corresponding control limit with a confidence level  $(1 - \alpha) \times 100\%$  is calculated as<sup>1,27</sup>

$$\delta^2 = g \cdot \chi_\alpha^2(h)\tag{5}$$

where  $g = \theta_2/\theta_1$ ,  $h = \theta_1^2/\theta_2$ , and  $\theta_1 = \sum_{i=l+1}^m \lambda_i$ ,  $\theta_2 = \sum_{i=l+1}^m \lambda_i^2$ , here  $\lambda_i$  is the  $i$ th largest eigenvalue of the covariance matrix  $\mathbf{S}$ . The *SPE* measures the deviation from  $\mathbf{x}$  to the PCS,

which represents the main correlation of the variables. Therefore, large deviation means a significant change in the correlation of the variables.

The Hotelling's  $T^2$ , characterizes the variation of the normal samples in the PCS, is defined as

$$T^2(\mathbf{x}) = \left\| \mathbf{\Lambda}^{-\frac{1}{2}} \mathbf{P}^T \mathbf{x} \right\|^2 = \mathbf{x}^T \mathbf{D} \mathbf{x} \quad (6)$$

where  $\mathbf{D} = \mathbf{P} \mathbf{\Lambda}^{-1} \mathbf{P}^T$  is symmetric and positive semi-definite. The corresponding control limit  $\tau^2$  with a confidence level  $(1 - \alpha) \times 100\%$  can be approximated by a chi-square distribution  $\chi_\alpha^2(l)$  when  $n$  is large enough<sup>26</sup>.

Yue and Qin<sup>6</sup> proposed an index,  $\varphi$ , that combines  $SPE$  and  $T^2$

$$\varphi(\mathbf{x}) = \mathbf{x}^T \mathbf{\Phi} \mathbf{x} = \frac{SPE}{\delta^2} + \frac{T^2}{\tau^2} \quad (7)$$

where  $\mathbf{\Phi} = \tilde{\mathbf{C}}/\delta^2 + \mathbf{D}/\tau^2$ . The control limit of  $\varphi$  with a confidence level  $(1 - \alpha) \times 100\%$  is

$$\zeta^2 = g_\varphi \cdot \chi_\alpha^2(h_\varphi) \quad (8)$$

where  $g_\varphi = \frac{1/\tau^4 + \theta_2/\delta^4}{1/\tau^2 + \theta_1/\delta^2}$ ,  $h_\varphi = \frac{(1/\tau^2 + \theta_1/\delta^2)^2}{1/\tau^4 + \theta_2/\delta^4}$ .

Note that the above detection indices can be written into a unified quadratic form<sup>9,21</sup>

$$\text{Index}(\mathbf{x}) = \left\| \mathbf{M}^{1/2} \mathbf{x} \right\|^2 = \mathbf{x}^T \mathbf{M} \mathbf{x} \quad (9)$$

The general quadratic detection index becomes the  $SPE$ ,  $T^2$ , and combined index  $\varphi$ , when  $\mathbf{M}$  is equal to  $\tilde{\mathbf{C}}$ ,  $\mathbf{D}$ , and  $\mathbf{\Phi}$ , respectively.

## Fault diagnosis based on reconstruction method

This section briefly describes the fault diagnosis based on reconstruction method with combined index proposed by Yue and Qin,<sup>6</sup> which can be considered as a representative recon-



struction method.

The task of fault reconstruction is to estimate the normal part of the faulty sample  $\mathbf{x}$ , i.e.,  $\mathbf{x}^*$ , by eliminating the effect of the fault on the detection indices. If the direction or subspace in which the fault occurred is already known, the reconstruction can be easily done. However, the true fault subspace is usually unknown in practice. So we have to check a set of the possible fault subspaces, and find out which is the real one.

It is assumed that a fault occurs in one of the possible fault subspaces from the set  $\mathcal{F} = \{\Xi_j \in \mathbb{R}^{m \times l_j}, j = 1, \dots, L\}$ , a reconstructed sample  $\mathbf{x}_j$  is an adjustment of the faulty sample vector,  $\mathbf{x}$ , along a assumed fault direction  $\Xi_j$

$$\mathbf{x}_j = \mathbf{x} - \Xi_j \mathbf{f}_j \quad (10)$$

where  $\mathbf{f}_j$  is to be estimated such that  $\mathbf{x}_j$  is closest to the normal region. The “closest” is modeled by minimizing the detection statistic of the reconstructed sample vector  $\mathbf{x}_j$

$$\min_{\mathbf{f}_j} \varphi(\mathbf{x}_j) \quad (11)$$

The detection statistic  $\varphi(\mathbf{x}_j)$  should be within the normal control region, i.e.  $\varphi(\mathbf{x}_j) \leq \zeta^2$ , if the assumed subspace  $\Xi_j$  is the true fault subspace. The estimated fault magnitude, which is the solution of the optimization problem defined in (11), is

$$\hat{\mathbf{f}}_j = \arg \min_{\mathbf{f}_j} \varphi(\mathbf{x}_j) = (\Xi_j^T \Phi \Xi_j)^{-1} \Xi_j^T \Phi \mathbf{x} \quad (12)$$

If the fault can only be reconstructed back into the normal region along one of the fault subspaces, then the true fault subspace can be uniquely identified. Otherwise, the fault subspace cannot be easily determined.

Yue and Qin proved that the reconstructed sample vector  $\mathbf{x}_j$  and estimated  $\mathbf{f}_j$  are unbiased estimation of the vector  $\mathbf{x}^*$  and  $\mathbf{f}$  respectively, if the true fault subspace is chosen for

reconstruction.<sup>6</sup>

## Analysis of Reconstruction Method for Fault Diagnosis

As mentioned in the previous section, the idea of reconstruction method is to modify the fault sample vector along a possible fault subspace and then determine the fault subspace by evaluating the detection index of the reconstructed sample. It is easy to understand that the faulty sample can be reconstructed back into the normal region if the true fault subspace is used in the reconstruction. However, in some cases the true fault subspace is not the only one that can bring the faulty sample back into the normal region. We will show that faulty samples can be brought back into the normal region even though reconstructing using other non-faulty subspaces.

### A special case

We assume that a faulty sample  $\mathbf{x}$  lies in a subspace  $\Xi_j$ , which is caused by a fault with its directions  $\Xi_i$  ( $\Xi_i \neq \Xi_j$ ) and magnitude  $\mathbf{f}$  ( $\mathbf{x} = \mathbf{x}^* + \Xi_i \mathbf{f}$ ). When the true fault subspace  $\Xi_i$  is chosen for reconstruction, the faulty sample  $\mathbf{x}$  can be reconstructed back into the normal region. However, the reconstructed sample vector  $\mathbf{x}_i$  and the estimated  $\mathbf{f}_i$  may not equal to the original normal sample vector  $\mathbf{x}^*$  and the fault magnitude  $\mathbf{f}_i$ , respectively, because  $\varphi(\mathbf{x}_i)$  is the minimum according to the reconstruction formula, but  $\varphi(\mathbf{x}^*)$  may not be, i.e.,  $\varphi(\mathbf{x}^*) \geq \varphi(\mathbf{x}_i)$ .

However, the direction  $\Xi_i$  is not the only one that can bring the faulty sample  $\mathbf{x}$  back into the normal region. In this case, the faulty sample  $\mathbf{x}$  can also be reconstructed back into the normal region if the subspace  $\Xi_j$  is chosen for reconstruction. More specifically, the reconstruct sample vector  $\mathbf{x}_j$  is exactly equal to the origin, i.e.,  $\mathbf{x}_j = \mathbf{0}$ , thus any of those detection statistics of  $\mathbf{x}_j$  are also equal to zero, e.g.,  $\varphi(\mathbf{x}) = 0 < \zeta^2$ . This is because the faulty sample  $\mathbf{x}_j$  belongs to the column space of  $\Xi_j$ , i.e.,  $\mathbf{x}_j \in \mathcal{N}(\Xi_j)$ , thus we can find an

unique linear representation of  $\mathbf{x}$  in  $\Xi_j$ , i.e.,  $\mathbf{x} = \Xi_j \mathbf{b}$ . Moreover, the optimal solution of fault magnitude,  $\mathbf{f}_j$ , is equal to the vector  $\mathbf{b}$  if reconstructing through the subspace  $\Xi_j$ .

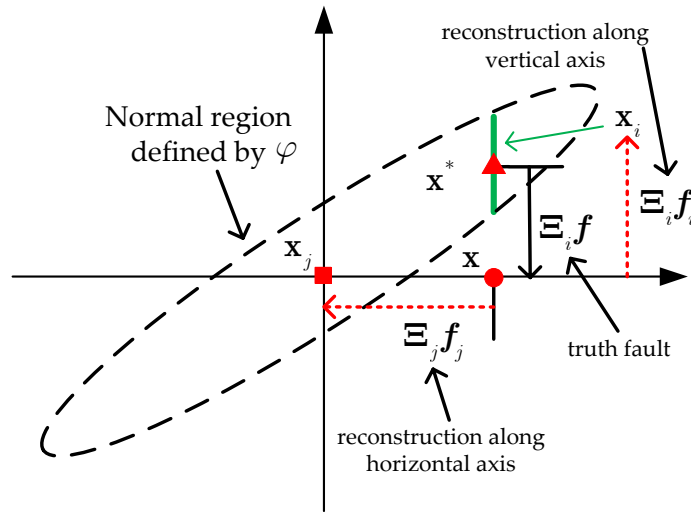


Figure 1: The illustrative example of fault identification

the true fault subspace since the reduced detection index of the subspace  $\Xi_i$  is not always smaller than that of the subspace  $\Xi_j$ .

## Small fault magnitude

**A fault affecting one or several measured variables simultaneously can cause a significant change in the correlation of the variables while the  $T^2$  index is still in control.** That is to say the *SPE* index of the measurements exceed its control limit while the  $T^2$  index does not exceed its control limit. This kind of fault may be reconstructed by either the true faulty subspace or the other non-faulty subspaces, because the variable correlation is possible to be recovered by modifying either faulty variables or the other non-faulty variables.

The *SPE* index of the reconstructed sample  $\mathbf{x}_j$  is

$$\begin{aligned}
SPE(\mathbf{x}_j) &= \|\tilde{\mathbf{C}}\mathbf{x}_j\|^2 \\
&= \|\tilde{\mathbf{C}}(\mathbf{x} - \Xi_j\mathbf{f}_j)\|^2 \quad (\mathbf{x}_j = \mathbf{x} - \Xi_j\mathbf{f}) \\
&= \|\tilde{\mathbf{C}}\mathbf{x} - \tilde{\mathbf{C}}\Xi_j\mathbf{f}_j\|^2 \\
&= \|\tilde{\mathbf{C}}(\mathbf{x}^* + \Xi_i\mathbf{f}_i) - \tilde{\mathbf{C}}\Xi_j\mathbf{f}_j\|^2 \quad (\mathbf{x} = \mathbf{x}^* + \Xi_i\mathbf{f}) \\
&= \|\tilde{\mathbf{C}}\mathbf{x}^* + \tilde{\mathbf{C}}(\Xi_i\mathbf{f} - \Xi_j\mathbf{f}_j)\|^2
\end{aligned} \tag{13}$$

If the true fault subspace  $\Xi_i$  is chosen for reconstruction, i.e.,  $\Xi_j = \Xi_i$ , then with an appropriate estimated  $\mathbf{f}_j$ , i.e.,  $\mathbf{f}_j = \mathbf{f}$ , the second part in the last equation of (13),  $\Xi_i\mathbf{f} - \Xi_j\mathbf{f}_j$ , will equal to or approach to zero. Thus, the *SPE* index of the reconstructed sample  $\mathbf{x}_j$  must be smaller than its control limit.

However, the true faulty subspace  $\Xi_i$  in this case may not be the unique subspace that can bring the faulty sample back into the normal region. Other non-fault subspaces may also bring the faulty sample back into the normal region, even if the assumed subspace  $\Xi_j$  used for reconstruction is totally different from the true fault subspace, i.e.,  $\Xi_j \perp \Xi_i$ . In this

case, equation (13) can be written as

$$\begin{aligned} SPE(\mathbf{x}_j) &= \left\| \tilde{\mathbf{C}}\mathbf{x}^* + \tilde{\mathbf{C}}(\Xi_i \mathbf{f} - \Xi_j \mathbf{f}_j) \right\|^2 \\ &= \left\| \tilde{\mathbf{C}}\mathbf{x}^* + \tilde{\mathbf{C}} \cdot [\Xi_i \ \Xi_j] \cdot [\mathbf{f}^T - \mathbf{f}_j^T]^T \right\|^2 \end{aligned} \quad (14)$$

When the subspace  $\Xi_i$  and  $\Xi_j$  orthogonal complement spaces, i.e.,  $\dim(\Xi_i) + \dim(\Xi_j) = m$ , where  $\dim(\cdot)$  represents the dimension of the corresponding subspace. In this case, the matrix  $[\Xi_i \ \Xi_j]$  can be obtained by exchanging the columns of the  $m \times m$  identity matrix. Hence, the equation (14) can be written as

$$SPE(\mathbf{x}_j) = \left\| \tilde{\mathbf{C}}\mathbf{x}^* + \tilde{\mathbf{C}}_{ij} \cdot [\mathbf{f}^T - \mathbf{f}_j^T]^T \right\|^2 \quad (15)$$

where,  $\tilde{\mathbf{C}}_{ij} = \tilde{\mathbf{C}} \cdot [\Xi_i \ \Xi_j]$  is obtained by exchanging the columns of the matrix  $\tilde{\mathbf{C}}$  according to the order defined by  $[\Xi_i \ \Xi_j]$ . If the vector  $[\mathbf{f}^T - \mathbf{f}_j^T]^T$  (with an appropriately estimated vector  $-\hat{\mathbf{f}}_j^T$ ) is perpendicular to the subspace spanned by the columns of  $\tilde{\mathbf{C}}_{ij}$ , the second component in the right hand side of the equation (15) will equal to zero, thus guaranteeing  $SPE(\mathbf{x}_j) \leq \delta_\alpha^2$ . This could happen with high probability when the fault affects few sensors or variables. In this situation, the degrees of freedom for estimating the vector  $-\mathbf{f}_j^T$  could be high and the feasible solution space for  $-\mathbf{f}_j^T$  is bigger, so it is easier to find a appropriate solution.

When  $\dim(\Xi_i) + \dim(\Xi_j) = \bar{m} < m$ , the matrix  $[\Xi_i \ \Xi_j]$  can be extended as  $[\Xi_i \ \Xi_j \ \mathbf{A}]$ , where the auxiliary matrix  $\mathbf{A}$  ( $\dim(\mathbf{A}) = m - \bar{m}$ ) is composed of the columns of the identity matrix. Then the equation (14) can be written as

$$\begin{aligned} SPE(\mathbf{x}_j) &= \left\| \tilde{\mathbf{C}}\mathbf{x}^* + \tilde{\mathbf{C}}(\Xi_i \mathbf{f} - \Xi_j \hat{\mathbf{f}}_j) \right\|^2 \\ &= \left\| \tilde{\mathbf{C}}\mathbf{x}^* + \tilde{\mathbf{C}} \cdot [\Xi_i \ \Xi_j] \cdot [\mathbf{f}^T \ \mathbf{f}_j^T]^T \right\|^2 \\ &= \left\| \tilde{\mathbf{C}}\mathbf{x}^* + \tilde{\mathbf{C}} \cdot [\Xi_i \ \Xi_j \ \mathbf{A}] \cdot [\mathbf{f}^T - \mathbf{f}_j^T \ \mathbf{0}^T]^T \right\|^2 \end{aligned}$$

$$= \left\| \tilde{\mathbf{C}}\mathbf{x}^* + \tilde{\mathbf{C}}_{ijA} \cdot [\mathbf{f}^T - \mathbf{f}_j^T \mathbf{0}^T]^T \right\|^2 \quad (16)$$

where,  $\tilde{\mathbf{C}}_{ijA} = \tilde{\mathbf{C}} \cdot [\mathbf{\Xi}_i \ \mathbf{\Xi}_j \ \mathbf{A}]$  is obtained by exchanging the columns of the matrix  $\tilde{\mathbf{C}}$  according to the order defined by  $[\mathbf{\Xi}_i \ \mathbf{\Xi}_j \ \mathbf{A}]$ . Similarly, if the vector  $[\mathbf{f}^T - \mathbf{f}_j^T \mathbf{0}^T]^T$  (with an appropriately estimated vector  $-\hat{\mathbf{f}}_j^T$ ) is perpendicular to the subspace spanned by the columns of  $\tilde{\mathbf{C}}_{ijA}$ , the second component in the right hand side of the equation (15) will equal to zero, thus guaranteeing  $SPE(\mathbf{x}_j) \leq \delta_\alpha^2$ . In this situation, compared with the problem defined in equation (14), the degree of freedom for estimating the vector  $-\mathbf{f}_j^T$  is lower and the feasible solution space for  $-\mathbf{f}_j^T$  is also smaller, but it is still possible to find a appropriate solution.

According to the above analysis, it can be seen that the PCA-based reconstruction method cannot uniquely identify the true faulty subspace with high probability when the true fault magnitude  $\mathbf{f}$  is small. However, if the true fault has a larger magnitude that causes the  $T^2$  exceeding its control limit, the combined index of the faulty samples in this case cannot be reconstructed back into the normal region through the non-faulty subspace, because the non-faulty subspace based reconstruction can only recover the variable correlation (i.e.,  $SPE$ ). The  $T^2$  index of the reconstructed sample still exceeds its control limit, so the combined index cannot be reconstructed back into the normal region as well.

## Numerical Simulation

In this section, a numerical simulation is used to demonstrate our view on combined index based reconstruction method. The normal operating condition (NOC) data is generated

according to the following model<sup>4</sup>

$$\mathbf{x} = \begin{bmatrix} -0.3441 & 0.4815 & 0.6637 \\ -0.2313 & -0.5936 & 0.3545 \\ -0.5060 & 0.2495 & 0.0739 \\ -0.5552 & -0.2405 & -0.1123 \\ -0.3371 & 0.3822 & -0.6115 \\ -0.3877 & -0.3868 & -0.2045 \end{bmatrix} \begin{bmatrix} t_1 \\ t_2 \\ t_3 \end{bmatrix} + noise \quad (17)$$

where random variables  $t_1$ ,  $t_2$ , and  $t_3$  are uniformly distributed in the range of  $[0, 1]$ ,  $[0, 1.6]$ , and  $[0, 1.2]$ , respectively. The noise is normally distributed with zero-mean and a standard deviation of 0.02. The number of data samples generated for training and validation are 2000 and 1000 respectively. The training data, which are scaled to zero-mean and unit variance, are used to construct the PCA model. The number of selected principle components is three which gives the accumulated contribution of 99.81%. The validation data are used to adjust control limits in order to ensure that the false alarm rate on normal data is no larger than a tolerance level  $\alpha$  ( $\alpha = 0.01$ ).

In order to illustrate the ability of reconstruction-based method for fault identification, three simulation examples are conducted. In these three examples, additional 100 normal data samples are generated and different kinds of faults are added on them.

In example 1, sensor 1 has a constant deviation with a magnitude 0.3, i.e.,  $\Xi_i = [\mathbf{e}_1]$ ,  $\mathbf{f} = 0.3$ , where  $\mathbf{e}_1$  represents the first column of the identity matrix. The fault detection results based on the PCA model are shown in Figure 2. Due to the small fault on sensor 1, the variables correlation is changed. This is reflected by the  $SPE$  shown in the upper plot of Figure 2. The  $SPE$  index of these fault data exceed its control limit  $\delta^2$ . However, this small fault does not cause a significant change in the  $T^2$  index. So, the  $T^2$  index of these fault data are below its control limits, which can be seen in the middle plot of Figure 2. Therefore, as a combination of the  $SPE$  and  $T^2$  index, the combined index-based plot in the bottom of

Figure 2 also indicates an abnormal behavior.

To identify the fault subspace, the reconstruction based method is used in this example. By inspecting the projection matrix  $\tilde{\mathbf{C}}$  in this example, variable 3 and variable 6 are most correlated with variable 1. So, reconstructions using the true subspace  $\Xi_i = [\mathbf{e}_1]$  and the subspace  $\Xi_j = [\mathbf{e}_3, \mathbf{e}_6]$  are compared. The fault detection results of the reconstructed samples are shown in Figure 3. After the reconstruction using both of the two subspaces, the effect of the fault was eliminated. If more correlated variables are used in the reconstruction, the more candidates of the fault subspace will be available. Hence, at least two candidates of the subspaces are identified as the possible fault subspace in this example. Although the sensor validation index suggested by Dunia et al.<sup>19</sup> can be used for further identification, no identical conclusion can be obtained, because the reduction amount in the detection indices of the reconstructed samples using  $\Xi_i$  is not always smaller than that of the reconstructed samples using  $\Xi_j$ .

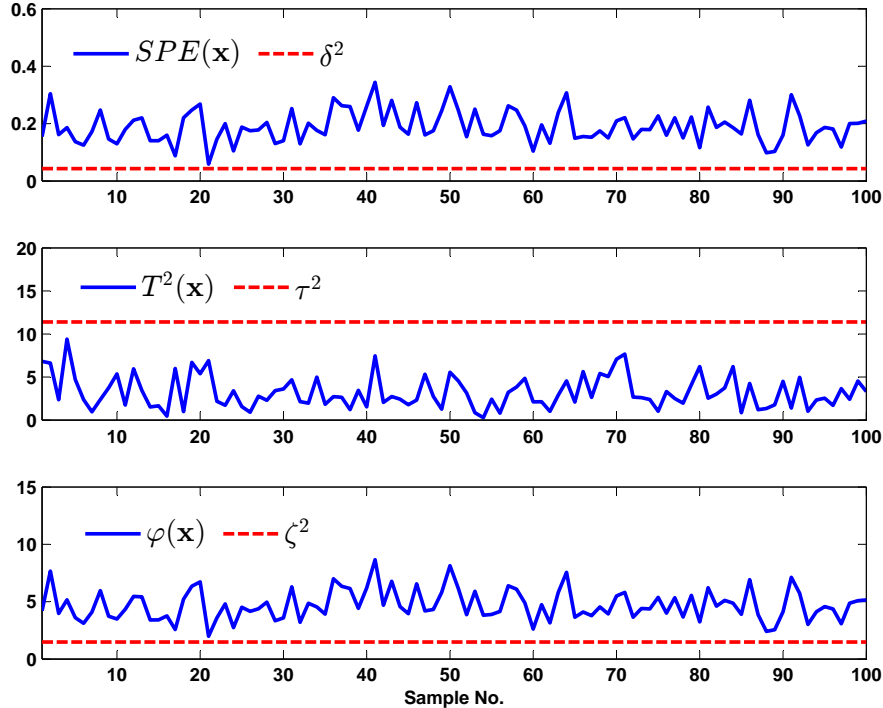


Figure 2: Fault detection results of example 1

Example 2 is used to illustrate the special case discussed in the previous section. It



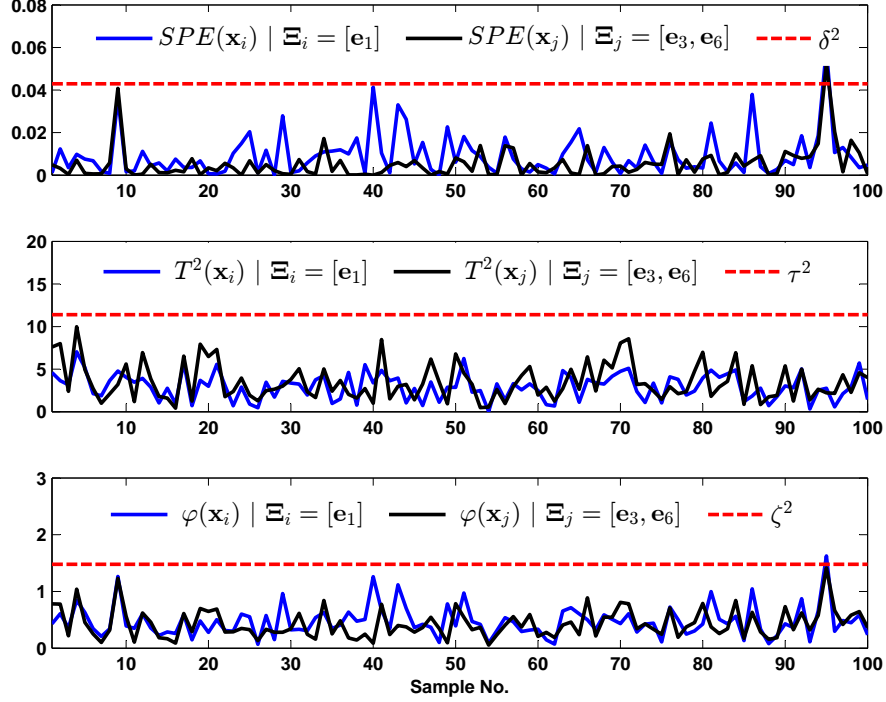


Figure 3: Fault reconstruction results of example 1

is assumed that the faults occur on three sensors (i.e., sensor 2, sensor 3, and sensor 6) and cause the outputs of the three sensors being always equal to the means of these three variables on the training data, respectively. Hence, the simulated fault samples have the same fault subspace, i.e.,  $\Xi_i = [\mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_6] \in \mathbb{R}^{6 \times 3}$ , where  $\mathbf{e}_j$ ,  $j = 2, 3, 6$  represents the  $j$ th column of the identity matrix. The fault magnitudes are small since the measurements of the normal samples vary around their means. In addition, these fault sample vectors after scaling are all located in a subspace spanned by  $\Xi_j = [\mathbf{e}_1, \mathbf{e}_4, \mathbf{e}_5]$  (i.e., the values of variables 2, 3, and 6 are all equal to zero after auto-scaling). Obviously, the subspaces  $\Xi_i$  and  $\Xi_j$  are orthogonal complements in this case. Due to the faults on sensors 2, 3, and 6, the variable correlations are changed. The fault detection results shown in Figure 4 also demonstrate this. The  $SPE$  index of all the fault samples exceed its control limit and the  $T^2$  index of all the fault samples are below its control limit. The combined index-based plot shown in the bottom of Figure 4 also indicates the existence of a fault.

To validate previous analysis, two subspaces, i.e., the true fault subspace  $\Xi_i = [\mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_6]$

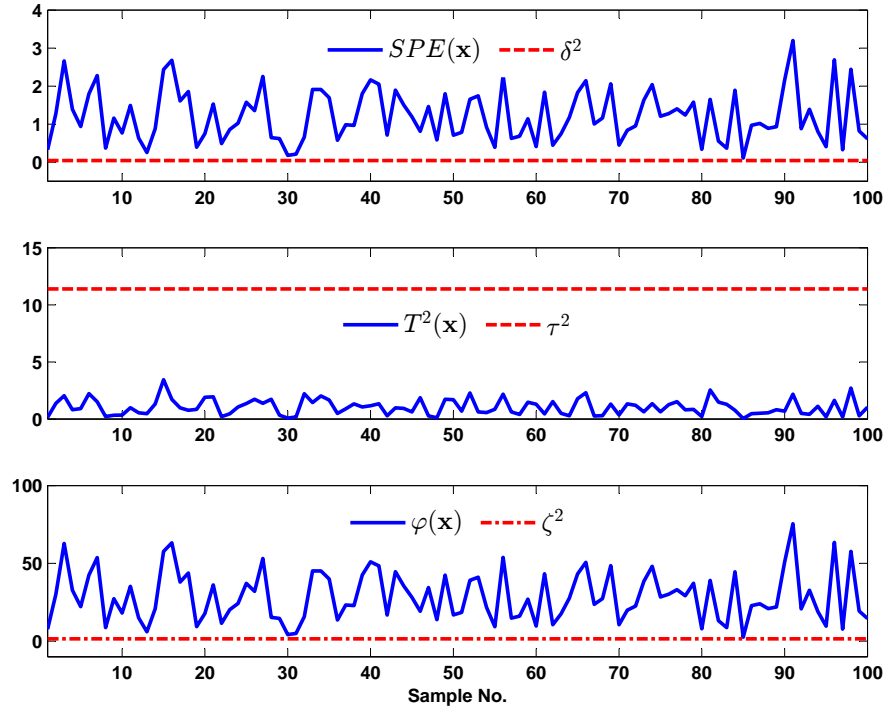


Figure 4: Fault detection results of example 2

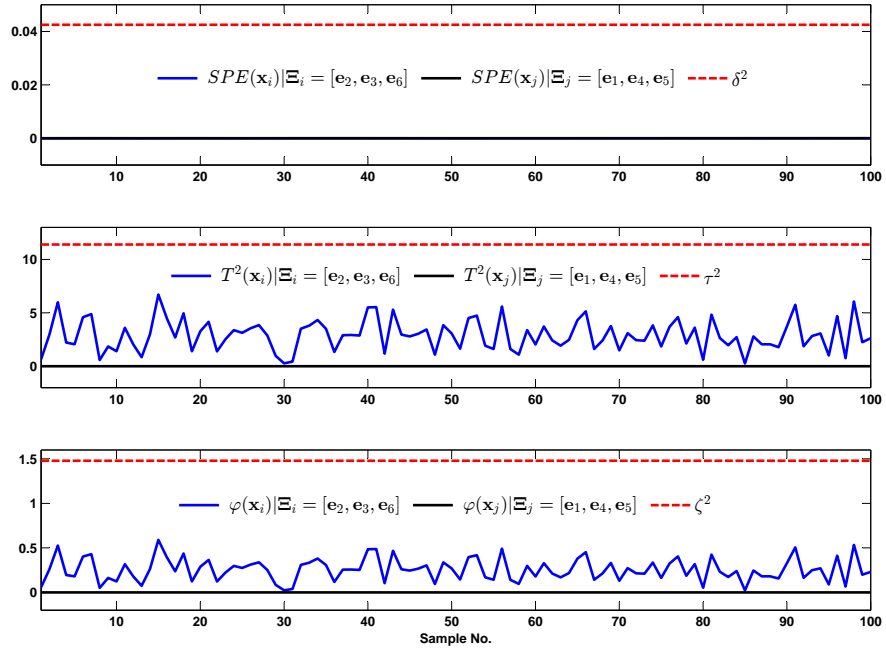


Figure 5: Fault reconstruction results of example 2

and its complementary subspace  $\Xi_j = [\mathbf{e}_1, \mathbf{e}_4, \mathbf{e}_5]$ , are used in the reconstruction-based fault identification. The fault detection results of the reconstructed samples are compared in Figure 5. The reconstruction based on either the true fault subspace  $\Xi_i$  or its complementary subspace  $\Xi_j$  can bring the faulty samples back into the normal region. It can also be seen that the reconstructed sample vectors using the complementary subspace  $\Xi_j$  are exactly the origin, which is identical to the previous theoretical analysis. In addition, the SVI using the non-faulty subspace  $\Xi_j$  is obviously small than that of using the true fault subspace  $\Xi_i$ . Therefore, it cannot easily identify the true fault subspace of these faulty samples in this case.

In example 3, a fault is also added on sensor 1, but with a large magnitude of 3. This significant change in the sensor output results in dramatic increases of those fault detection indices shown in Figure 6. To identify the fault subspace, the true fault subspace  $\Xi_i = [\mathbf{e}_1]$  and the subspace  $\Xi_j = [\mathbf{e}_3, \mathbf{e}_5, \mathbf{e}_6]$  are used for fault reconstruction. It can be seen that only the true fault subspace can reconstruct the normal samples. For the subspace  $\Xi_j = [\mathbf{e}_3, \mathbf{e}_5, \mathbf{e}_6]$ , although the correlation of the variables can be reconstructed, the  $T^2$  index cannot be reduced below its control limit through reconstruction. Thus, the combined index-based plot in the bottom of Figure 7 still indicates the existence of the fault after the reconstruction by the non-faulty subspace.

## Conclusions and Discussions

In this paper, we review the PCA-based method for statistical process monitoring. For the fault diagnosis without any historical fault data, two kinds of representative methods can be used: contribution analysis methods and reconstruction-based method. The ability of the reconstruction method for identifying fault subspace is analysed. The theoretical analysis and numerical simulation are used to show that the reconstruction method cannot uniquely identify the true fault subspace in some cases. In spite of this, the idea of the

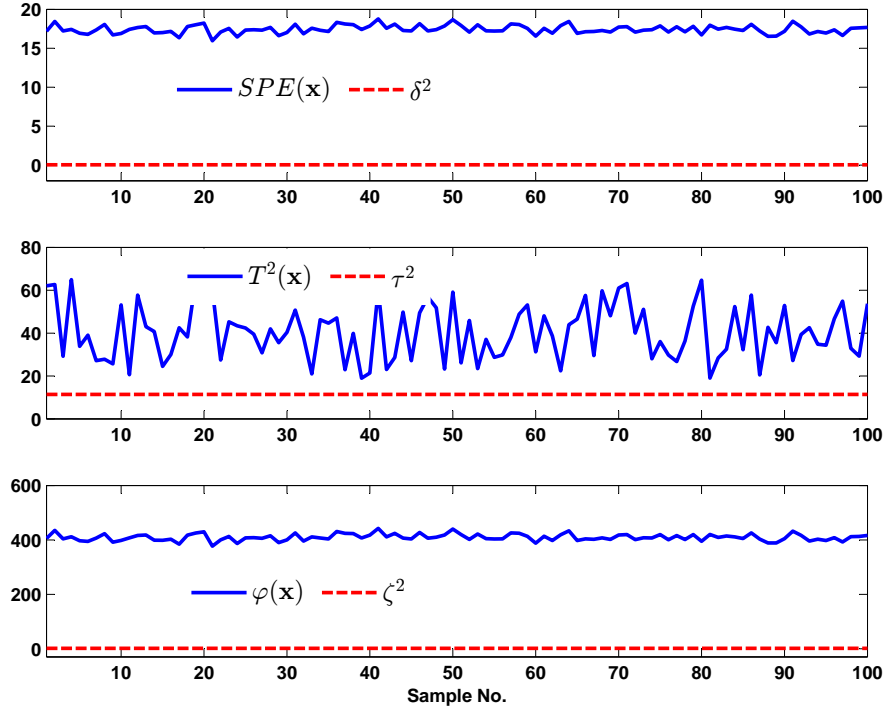


Figure 6: Fault detection results of example 3

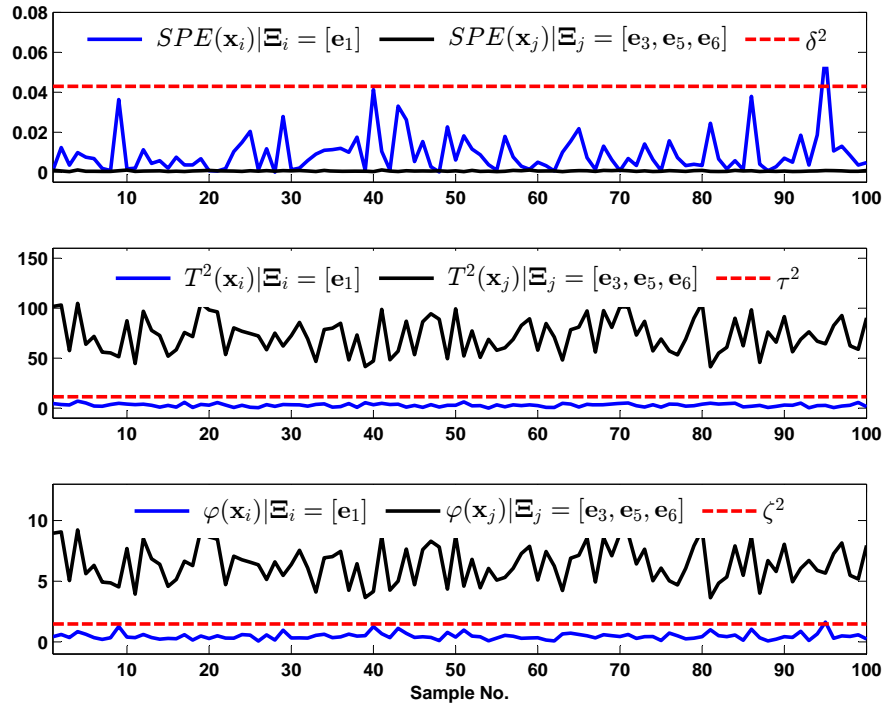


Figure 7: Fault reconstruction results of example 3

reconstruction based method for fault diagnosis is useful and its effectiveness can be seen from many successful industrial applications.

This kind of problem is prone to occur when a fault occurred and affected one or several measured variables simultaneously causing a significant change in the correlation of the variables while the  $T^2$  index does not exceed its control limit. As Qin<sup>26</sup> stated, a fault is easier to cause the measurement sample exceeding its *SPE* control limit rather than  $T^2$  control limit because the normal region defined by the control limit of  $T^2$  is usually much larger than that defined by the control limit of *SPE*. Therefore, this kind of fault occurs frequently, which can be seen from the experimental results of process monitoring in the published literatures<sup>28</sup>. Reconstruction of either the faulty sensors or other non-faulty sensors can recover the correlation of the variables. From the simulation results, the reconstruction using the non-fault subspace always modify more measurements than that of using the true fault subspace. Hence, the difference between the reconstructed sample and the original faulty sample can used as an auxiliary index for fault subspace identification. Furthermore, the dynamical information from the previous normal process measurements may also be used for further identification, because, for a steady dynamical process, the difference of measurements from close sampling times is small. The distance between the reconstructed sample and the measurement sample from previous sampling times can be used as an auxiliary indicator for helping identify the fault subspace if similar situations occur.

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## Table of Contents (TOC) Graphic



